

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
 Data File : VU045098.D
 Acq On : 04 Oct 2021 15:59
 Operator : SY/MD
 Sample : M3996-06
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A22

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

Signal : TIC: VU045098.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	35	42	64	rBV2	167266	196267	0.93%	0.626%
2	1.601	74	81	94	rBV	142347	169096	0.80%	0.540%
3	1.909	169	177	195	rVB	117219	161389	0.76%	0.515%
4	2.469	343	351	360	rVB2	3651	5838	0.03%	0.019%
5	2.504	360	362	370	rVB3	257	253	0.00%	0.001%
6	2.569	370	382	403	rBV	234578	392252	1.85%	1.252%
7	2.733	430	433	440	rBV2	287	334	0.00%	0.001%
8	2.794	445	452	453	rBV	879	805	0.00%	0.003%
9	2.929	489	494	497	rBV	283	269	0.00%	0.001%
10	3.041	527	529	530	rBV	670	299	0.00%	0.001%
11	3.083	540	542	545	rVB3	461	226	0.00%	0.001%
12	3.128	554	556	558	rBV2	290	197	0.00%	0.001%
13	3.147	560	562	564	rVV	540	335	0.00%	0.001%
14	3.189	564	575	592	rVB2	4715	10180	0.05%	0.032%
15	3.321	612	616	619	rBV2	248	245	0.00%	0.001%
16	3.376	619	633	644	rVB4	3757	8179	0.04%	0.026%
17	3.479	662	665	668	rVV	192	164	0.00%	0.001%
18	3.507	671	674	677	rVV2	209	169	0.00%	0.001%
19	3.646	711	717	719	rVV2	213	242	0.00%	0.001%
20	3.659	719	721	724	rVV	186	155	0.00%	0.000%
21	3.835	774	776	779	rVB	234	151	0.00%	0.000%
22	3.932	802	806	808	rBV	187	155	0.00%	0.000%
23	3.996	819	826	829	rBV2	217	289	0.00%	0.001%
24	4.067	847	848	854	rVV2	199	208	0.00%	0.001%
25	4.244	898	903	907	rBV2	301	354	0.00%	0.001%
26	4.540	986	995	1002	rBV3	987	1631	0.01%	0.005%
27	4.630	1008	1023	1060	rBV	160399	426930	2.02%	1.362%
28	4.951	1117	1123	1127	rVB2	296	354	0.00%	0.001%
29	4.974	1127	1130	1134	rBV2	256	174	0.00%	0.001%
30	5.003	1136	1139	1142	rVB2	206	160	0.00%	0.001%
31	5.070	1142	1160	1183	rBV	220628	487708	2.30%	1.556%
32	5.221	1204	1207	1211	rVB3	438	337	0.00%	0.001%
33	5.266	1216	1221	1223	rBV	204	222	0.00%	0.001%
34	5.292	1223	1229	1237	rVB4	711	1248	0.01%	0.004%
35	5.331	1237	1241	1245	rBV2	225	273	0.00%	0.001%
36	5.388	1252	1259	1261	rBV2	555	669	0.00%	0.002%

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 Title : VOC Analysis

37	5.729	1343	1365	1398	rBV2	449500	1261325	5.96%	4.025%
38	5.900	1416	1418	1423	rVB2	393	337	0.00%	0.001%
39	5.993	1444	1447	1449	rBV2	212	172	0.00%	0.001%
40	6.102	1476	1481	1483	rBV2	160	185	0.00%	0.001%
41	6.253	1512	1528	1546	rBV	361719	679346	3.21%	2.168%
42	6.546	1607	1619	1632	rBV3	35830	68141	0.32%	0.217%
43	6.613	1637	1640	1642	rVB2	288	202	0.00%	0.001%
44	6.633	1642	1646	1649	rBV2	153	150	0.00%	0.000%
45	6.697	1649	1666	1690	rBV	293789	572872	2.71%	1.828%
46	6.806	1698	1700	1710	rVB6	886	1111	0.01%	0.004%
47	6.855	1710	1715	1719	rVB3	356	385	0.00%	0.001%
48	6.877	1719	1722	1729	rBV2	152	180	0.00%	0.001%
49	6.970	1746	1751	1755	rVB2	184	201	0.00%	0.001%
50	7.019	1762	1766	1769	rBV	175	176	0.00%	0.001%
51	7.038	1769	1772	1774	rBV	489	336	0.00%	0.001%
52	7.105	1789	1793	1794	rBV	633	390	0.00%	0.001%
53	7.186	1810	1818	1830	rVB4	2321	3985	0.02%	0.013%
54	7.568	1923	1937	1954	rBV	161696	284502	1.34%	0.908%
55	7.687	1967	1974	1984	rVB3	1928	3170	0.01%	0.010%
56	7.739	1986	1990	1994	rVB2	258	197	0.00%	0.001%
57	7.903	2027	2041	2054	rBV	532497	917679	4.34%	2.928%
58	7.974	2055	2063	2077	rVB	29802	51009	0.24%	0.163%
59	8.183	2114	2128	2148	rBV	111807	188346	0.89%	0.601%
60	8.482	2213	2221	2229	rBV2	470	844	0.00%	0.003%
61	8.559	2229	2245	2260	rBV	12743715	21166681	100.00%	67.544%
62	8.636	2261	2269	2299	rVB	531307	1002543	4.74%	3.199%
63	9.285	2465	2471	2479	rVB2	1013	1297	0.01%	0.004%
64	9.420	2499	2513	2548	rBV	509195	835261	3.95%	2.665%
65	9.575	2548	2561	2571	rVB	10841	16678	0.08%	0.053%
66	9.697	2590	2599	2611	rVV	10511	16684	0.08%	0.053%
67	9.854	2644	2648	2651	rBV	174	160	0.00%	0.001%
68	9.903	2660	2663	2666	rVB	276	195	0.00%	0.001%
69	9.983	2683	2688	2690	rBV	161	154	0.00%	0.000%
70	10.105	2717	2726	2736	rBV2	6698	9948	0.05%	0.032%
71	10.224	2758	2763	2764	rBV2	176	174	0.00%	0.001%
72	10.308	2784	2789	2792	rBV2	218	249	0.00%	0.001%
73	10.639	2889	2892	2897	rBV3	281	248	0.00%	0.001%
74	10.674	2897	2903	2915	rVB2	1991	2903	0.01%	0.009%
75	10.758	2915	2929	2949	rBV	418043	676142	3.19%	2.158%
76	10.864	2960	2962	2966	rBV2	180	156	0.00%	0.000%

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Min Area: 0 % of largest Peak

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

77	10.890	2966	2970	2972	rBV2	413	362	0.00%	0.001%
78	11.002	2999	3005	3009	rBV4	1326	1737	0.01%	0.006%
79	11.067	3022	3025	3027	rBV	282	218	0.00%	0.001%
80	11.096	3027	3034	3039	rVV2	1009	1286	0.01%	0.004%
81	11.295	3089	3096	3105	rVB3	578	961	0.00%	0.003%
82	11.472	3141	3151	3162	rBV2	7212	11584	0.05%	0.037%
83	11.700	3217	3222	3231	rVB2	823	885	0.00%	0.003%
84	11.816	3245	3258	3277	rBV	499467	790348	3.73%	2.522%
85	11.893	3277	3282	3285	rBV2	793	764	0.00%	0.002%
86	11.944	3292	3298	3301	rBV3	680	785	0.00%	0.003%
87	12.099	3339	3346	3353	rBV4	1473	2057	0.01%	0.007%
88	12.195	3364	3376	3401	rBV	527333	843989	3.99%	2.693%
89	12.356	3421	3426	3429	rBV2	255	325	0.00%	0.001%
90	12.639	3511	3514	3519	rVB3	270	223	0.00%	0.001%
91	12.973	3615	3618	3625	rVB3	395	422	0.00%	0.001%
92	13.057	3639	3644	3646	rBV2	200	197	0.00%	0.001%
93	13.456	3763	3768	3772	rBV3	724	827	0.00%	0.003%
94	14.089	3956	3965	3982	rVV	14244	23000	0.11%	0.073%
95	14.160	3985	3987	3990	rVB2	388	190	0.00%	0.001%
96	14.214	3996	4004	4012	rVB4	1490	2150	0.01%	0.007%
97	14.581	4113	4118	4124	rBV3	487	600	0.00%	0.002%
98	15.163	4296	4299	4300	rBV2	359	210	0.00%	0.001%
99	15.227	4310	4319	4335	rVB2	7380	12343	0.06%	0.039%
100	15.414	4368	4377	4388	rVB3	6201	9834	0.05%	0.031%

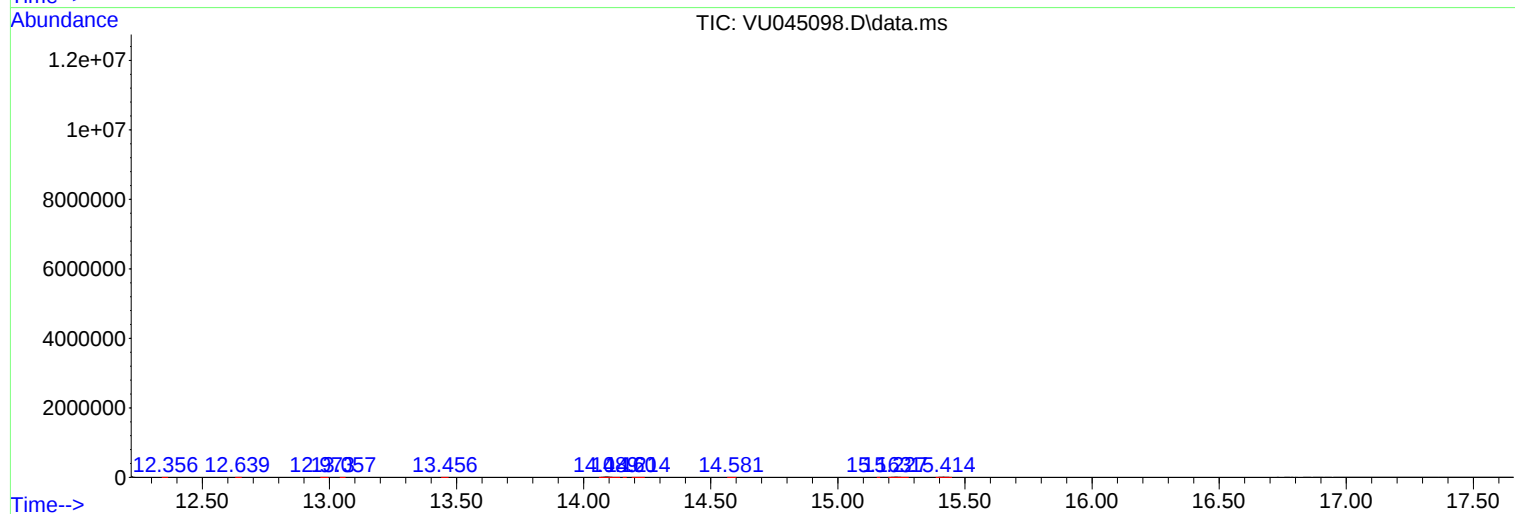
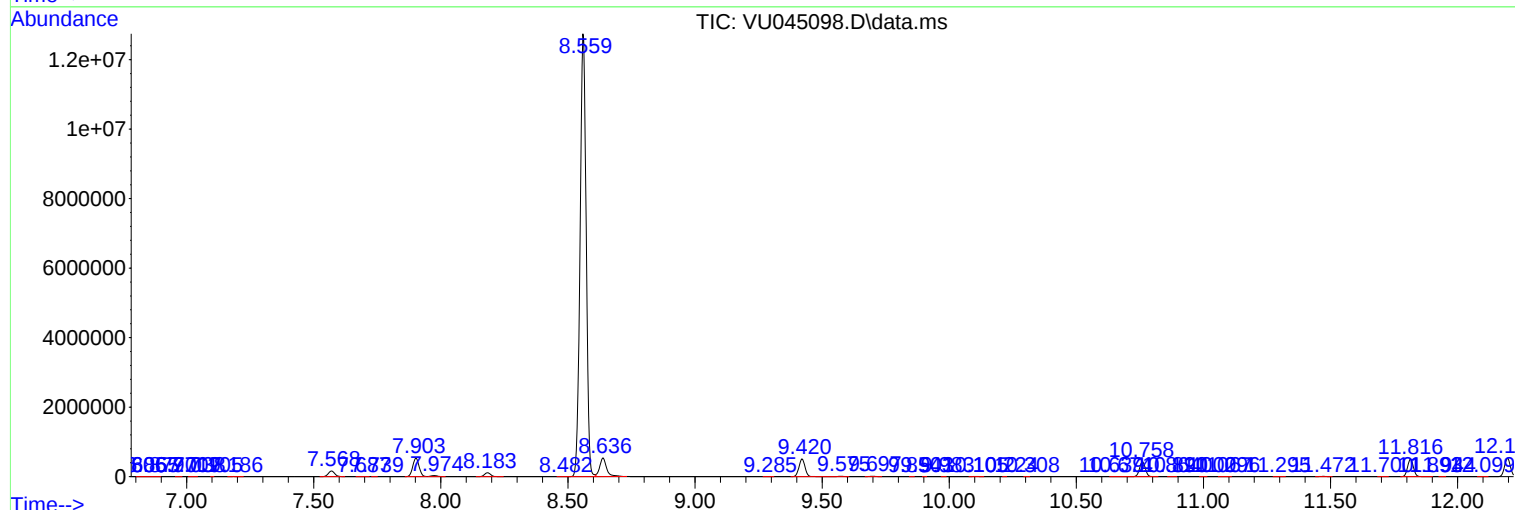
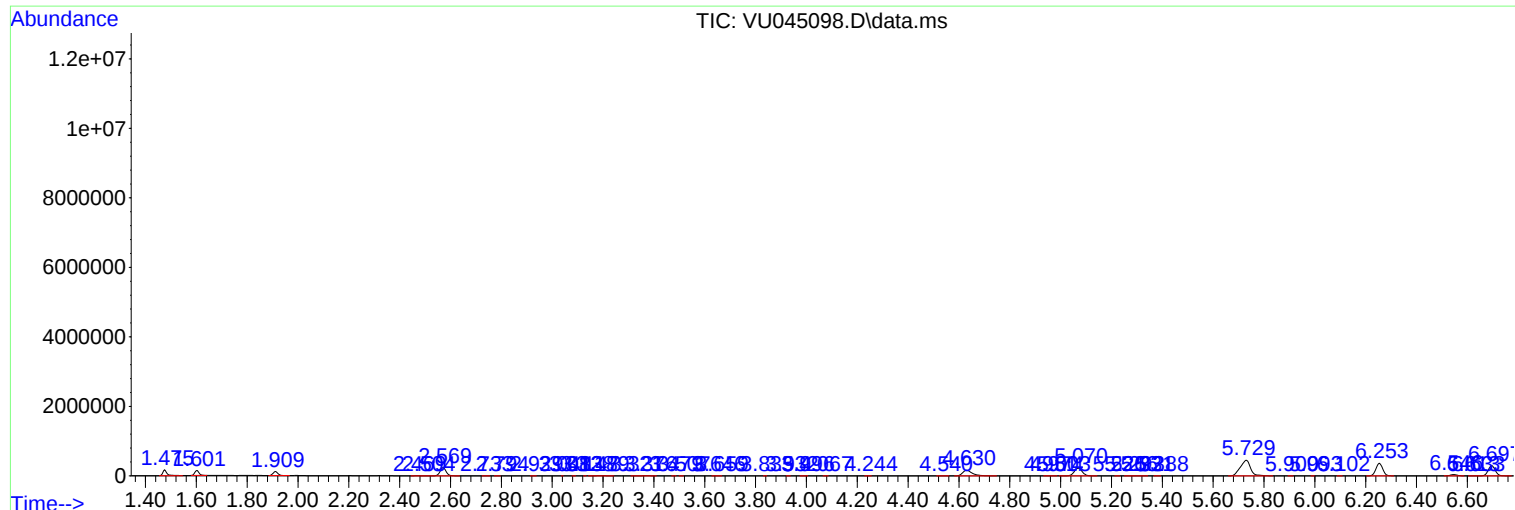
Sum of corrected areas: 31337768

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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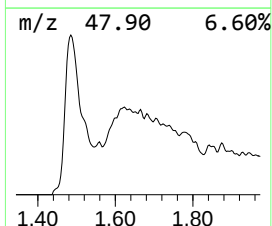
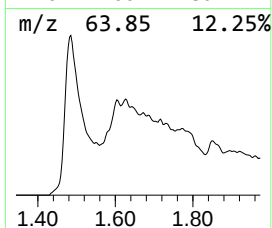
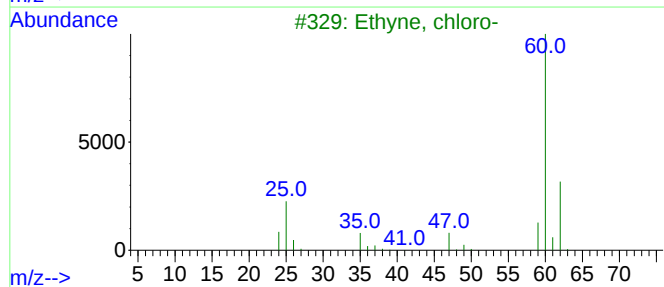
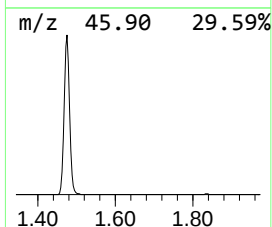
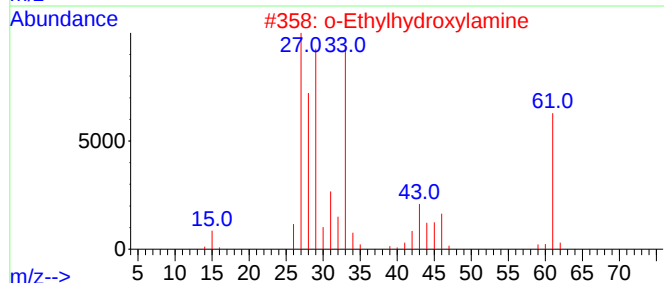
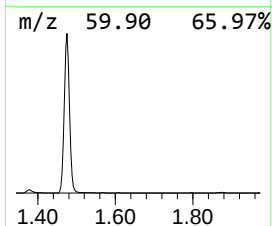
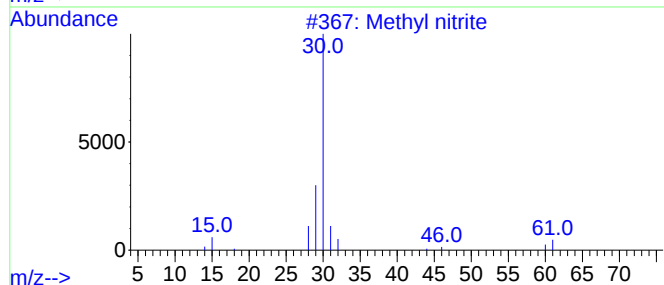
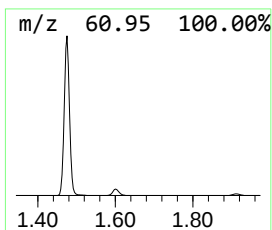
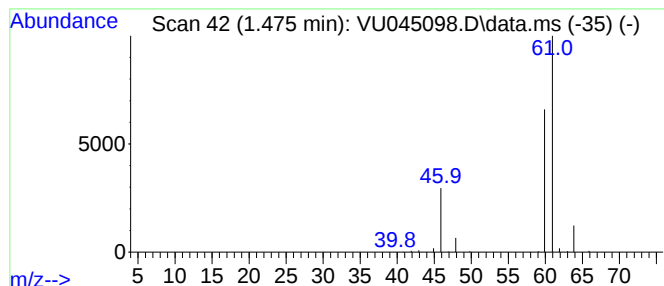
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	14.45 ug/L	196267	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl nitrite	61	CH3NO2	000624-91-9	5
2			o-Ethylhydroxylamine	61	C2H7NO	000624-86-2	4
3			Ethyne, chloro-	60	C2HCl	000593-63-5	4
4			Trifluoroguanidine	113	CH2F3N3	037950-72-4	4
5			Cyanogen chloride	61	CClN	000506-77-4	4



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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.475	14.4	ug/L	196267	1	6.253	679346	50.0